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Progress of Computational Machine Learning for Advancements in Nanoparticles and Nanomaterials

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As the technology in nanomedicines (NMs) and nano-particles (NPs) advance, coupled with creating advanced materials at the nanoscale, it‘s also a concern to know whether it‘s safe to use or not. Special attention must be paid toward safe design approaches for nanomaterial-based products. By using today‘s technology such as artificial intelligence (AI) and machine learning (ML) the understanding towards the topic can be increased by enhancing and improving the simulation and modeling process for nanotoxicology. The objective of this review is to know how Physiologically based pharmacokinetic (PBPK) modeling and absorption, distribution, metabolism, and excretion (ADME)-based in silico methods helps in finding the blind spots of nanotoxicity caused by the nanomedicines (NMs) and engineered nano-particles (ENPs). There are many computational tools (The computational OMICS, colloidal particle determination, and algorithms to establish dosimetry for inhalation toxicology, and quantitative structure–activity relationships at nanoscale (nano-QSAR)) that have assisted in finding toxic endpoints and different pathways taken by NMs and ENPs that can help in acceleration of clinical translation of these NMs and ENPs.